

Nuclear quadrupole moment of ^{43}Ca and hyperfine structure studies of its singly charged ion

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By combining our theoretical calculation and recently measured electric quadrupole hyperfine structure constant of the $3d\ 2D_{5/2}$ state in the singly ionized ^{43}Ca , we determine its nuclear quadrupole moment to one percent accuracy. The obtained result, $-0.0444(6)b$, is about ten percent improvement over the considered standard value. We have employed the relativistic coupled-cluster theory at single and double excitations level to calculate the electronic wave functions. The accuracy of these wave functions are estimated by comparing our calculated magnetic dipole hyperfine constants with their corresponding available experimental results of many low-lying states. We also present hyperfine structure constants for other higher excited states where experimental results are not reported. Role of the Breit interaction has been investigated in these properties.

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I. INTRODUCTION

Advanced modern techniques of laser cooling and trapping have enabled us to carry out precision measurements of hyperfine structure constants in atomic systems [1, 2]. Theoretical studies of these quantities require accurate many-body methods, inclusion of relativistic effects and knowledge of nuclear moments [3, 4, 5, 6]. Precise measurements of nuclear moments are difficult, especially the quadrupole and octupole moments. The prominent examples of techniques to measure them are NMR, atomic beams, optical pumping, recoil methods etc. [7, 8]. However, their absolute results are of great interest for the nuclear physicists to be able to test different nuclear models [9, 10]. The quadrupole moment of the stable isotope ^{43}Ca is also of particular interest in the evaluation of the nuclear magnetic resonance measurements in the biological systems [11, 12]. Investigating properties of nuclei in the region of magic numbers are challenging because the valence nucleons can be strongly affected by the close shell configuration. ^{43}Ca has mass number between the double magic numbers ^{40}Ca and ^{48}Ca suggesting peculiar nuclear charge distribution. It is plausible to obtain correct electronic wave functions, hence their properties, in the single valence atomic systems using the recently developed highly potential methods like all order relativistic coupled-cluster (RCC) theory [6, 13, 14, 15]. Singly ionized ^{43}Ca ($^{43}\text{Ca}^+$) is of medium size system and single and double excitations approximation RCC approach (CCSD method) is capable enough in such cases [13, 14, 15] to account electron correlation effects accurately. It has been observed that electron correlation effects exhibit spectacular behavior in the studies of the magnetic dipole hyperfine structure constant in the $2D_{5/2}$ states of the singly ionized alkaline-earth metal atoms. The CCSD method with contributions from lead-

ing order triple excitations (CCSD(T) method) is able to consider them sufficiently for which it can produce results matching with the precisely measured values [15, 16, 17]. In this work, we have used this method to evaluate the electronic matrix elements due to the hyperfine interaction operators.

It would also be imperative to mention here that $^{43}\text{Ca}^+$ is an interesting candidate for quantum computation [18] and optical frequency standard [19, 20]. Accurate values of hyperfine structure constants are useful in estimating shifts in the energy levels due to the stray electromagnetic fields during the experimental set-up [21, 22]. Again, theoretical estimations of these quantities are used to test the correct behavior of wave functions in the nuclear region [23, 24]. Nuclear magnetic moment of ^{43}Ca is known within sub-one percent accuracy [25], but its reported nuclear quadrupole moment values vary from $-0.0408(8)b$ to $-0.065(20)b$ [26, 27, 28, 29, 30]. Using the accurate matrix element of the electric quadrupole hyperfine interaction operator and precisely measured [31] electric quadrupole hyperfine structure constant of the $3d\ 2D_{5/2}$ state in $^{43}\text{Ca}^+$, we determine its nuclear quadrupole moment. Accuracy of the theoretical calculations are estimated from the analysis of the correct behavior of the wave functions which are able to reproduce the magnetic dipole hyperfine structure constants in a few low-lying states where experimental results are available. We also present hyperfine structure constants of other higher excited states for further testimony of our results using future experiments.

II. THEORY AND METHOD OF CALCULATIONS

The detail theory about the hyperfine structures are given earlier in a classic paper by C. Swartz [5]. Here, we have mentioned only these formulae in explicit form. The

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relativistic hyperfine interaction Hamiltonian is given by

$$H_{hfs} = \sum_l \mathbf{M}^{(l)} \cdot \mathbf{T}^{(l)} \quad (2.1)$$

where $\mathbf{M}^{(l)}$ and $\mathbf{T}^{(l)}$ are spherical tensor operators of rank l . In the first-order perturbation theory, hyperfine interaction energy W_F of the hyperfine state $|F; I, J\rangle$ of angular momentum $F = I + J$ with I and J being the nuclear spin and electronic angular momentum of the associated fine structure state $|J, M_J\rangle$, respectively, after neglecting terms beyond $l = 2$ is given by

$$W_F = \frac{1}{2} A_{hfs} K + B_{hfs} \frac{\frac{3}{2}K(K+1) - 2I(I+1)J(J+1)}{2I(2I-1)2J(2J-1)}, \quad (2.2)$$

where $K = F(F+1) - I(I+1) - J(J+1)$, A_{hfs} is the magnetic dipole structure constant for $l = 1$ and B_{hfs} is the electric quadrupole structure constant for $l = 2$. These constants are defined as

$$A_{hfs} = \mu_N g_I \frac{\langle J || \mathbf{T}^{(1)} || J \rangle}{\sqrt{J(J+1)(2J+1)}}, \quad (2.3)$$

and

$$B_{hfs} = Q_{nuc} \left\{ \frac{8J(2J-1)}{(2J+1)(2J+2)(2J+3)} \right\}^{1/2} \langle J || \mathbf{T}^{(2)} || J \rangle, \quad (2.4)$$

where we have used atomic unit (au). In the above expressions, μ_N is the Bohr magneton and we use $g_I = [\frac{\mu_I}{I}]$ with μ_I and $I(= 7/2)$ are the nuclear magnetic dipole moment and spin, respectively, as -0.37646943 from the measurement [25] to evaluate A_{hfs} . Since nuclear quadrupole moment, Q_{nuc} , is not known accurately, hence we calculate

$$\frac{B_{hfs}}{Q_{nuc}} = \left\{ \frac{8J(2J-1)}{(2J+1)(2J+2)(2J+3)} \right\}^{1/2} \langle J || \mathbf{T}^{(2)} || J \rangle. \quad (2.5)$$

The reduced matrix elements of the electronic spherical operators, $\mathbf{T}^{(l)} = \sum t^{(l)}$, in terms of single orbitals are given by

$$\langle \kappa_f || t^{(1)} || \kappa_i \rangle = -(\kappa_f + \kappa_i) \langle -\kappa_f || C^{(1)} || \kappa_i \rangle \int_0^\infty dr \frac{(P_f Q_i + Q_f P_i)}{r^2} \quad (2.6)$$

and

$$\langle \kappa_f || t^{(2)} || \kappa_i \rangle = -\langle \kappa_f || C^{(2)} || \kappa_i \rangle \int_0^\infty dr \frac{(P_f P_i + Q_f Q_i)}{r^3}, \quad (2.7)$$

where i and f represent initial and final orbitals, respectively. The reduced matrix elements of the spherical tensors ($C^{(l)}$) are given by

$$\langle \kappa_f || C^{(l)} || \kappa_i \rangle = (-1)^{j_f+1/2} \sqrt{(2j_f+1)(2j_i+1)} \begin{pmatrix} j_f & l & j_i \\ 1/2 & 0 & -1/2 \end{pmatrix} \pi(l_f, l, l_i) \quad (2.8)$$

with the angular momentum selection rule $\pi(l_f, l, l_i) = 1$ when $l_f + l + l_i = \text{even}$ for the orbital angular momenta l_f and l_i , otherwise zero.

The primary objective of this work is to calculate the above electronic matrix elements of the hyperfine interaction operators. It is obvious from the single particle expressions that these matrix elements have strong overlap with the nucleus. As a starting point, we consider kinetically balanced Gaussian type of orbitals (GTOs) which seem to be an ideal choice for obtaining correct behavior of wave functions in the nuclear region [32, 33] to calculate mean-field wave functions $|\Phi_0\rangle$ of the closed-shell configuration in the Dirac(Hartree)-Fock (DF) approach. To calculate the atomic state function (ASF) of single valence with closed-shell configurations, we express it in the RCC ansatz as

$$|\Psi_v\rangle = e^T \{1 + S_v\} |\Phi_v\rangle, \quad (2.9)$$

where $|\Phi_v\rangle$ is the new reference state which is defined as $|\Phi_v\rangle = a_v^\dagger |\Phi_0\rangle$ and will give the DF result for the above open-shell configuration. In the above expression, we call T and S_v as the closed and open shell core and core with valence electron excitation operators, respectively, which in the second quantization notation in the CCSD approximation are given by

$$T = T_1 + T_2 = \sum_{a,p} a_p^+ a_a t_a^p + \frac{1}{4} \sum_{ab,pq} a_p^+ a_q^+ a_b a_a t_{ab}^{pq}, \quad (2.10)$$

$$S_v = S_{1v} + S_{2v} = \sum_{p \neq v} a_p^+ a_v s_v^p + \frac{1}{2} \sum_{b,pq} a_p^+ a_q^+ a_b a_v s_{vb}^{pq} \quad (2.11)$$

where the $(a, b, c..)$, $(p, q, r..)$ and (v) subscripts of the second quantized operators represent core, particle (virtual) and valence orbitals, respectively. The t and s_v coefficients are the corresponding excitation amplitudes which are determined using the following equations

$$\langle \Phi^L | \{ \widehat{H_N e^T} \} | \Phi_0 \rangle = 0 \quad (2.12)$$

$$\langle \Phi_v^L | \{ \widehat{H_N e^T} \} S_v | \Phi_v \rangle = -\langle \Phi_v^L | \{ \widehat{H_N e^T} \} | \Phi_v \rangle + \langle \Phi_v^L | S_v | \Phi_v \rangle \Delta E_v \delta_L, \quad (2.13)$$

with the superscript $L(= 1, 2)$ representing the single and double excited states from the corresponding reference states and the wide-hat symbol denotes the linked terms. ΔE_v is the corresponding valence electron affinity energy which is evaluated by

$$\Delta E_v = \langle \Phi_v | \{ \widehat{H_N e^T} \} \{1 + S_v\} | \Phi_v \rangle. \quad (2.14)$$

In our CCSD(T) approach, we consider effects of the leading order triple excitations through ΔE_v by constructing triple excitation operator

$$S_{vbc}^{pqr} = \frac{\widehat{H_N T_2} + \widehat{H_N S_{v2}}}{\epsilon_b + \epsilon_c - \epsilon_r}, \quad (2.15)$$

and contracting S_{vbc}^{pqr} with the Hamiltonian to get contributions to the corresponding ΔE_v , where ϵ_i is the DF energy of the electron in the i^{th} orbital.

We consider the Dirac-Coulomb-Breit Hamiltonian in the above equations that is given by

$$H = c\vec{\alpha} \cdot \vec{p} + (\beta - 1)c^2 + V_{nuc}(r) + \frac{1}{r_{12}} - \frac{\vec{\alpha}_1 \cdot \vec{\alpha}_2}{r_{12}} + \frac{1}{2} \left\{ \frac{\vec{\alpha}_1 \cdot \vec{\alpha}_2}{r_{12}} - \frac{(\vec{\alpha}_1 \cdot \vec{r}_{12})(\vec{\alpha}_2 \cdot \vec{r}_{12})}{r_{12}^3} \right\} \quad (2.16)$$

where c is the velocity of light, α and β are the Dirac matrices and $V_{nuc}(r)$ is the nuclear potential. We solve the wave functions due to the above Hamiltonian in the DF and RCC methods self-consistently with the tolerance size below 10^{-7} to obtain precise results.

We evaluate expectation values due to the hyperfine interaction operators using our RCC method by

$$\begin{aligned} \langle O \rangle &= \frac{\langle \Psi_v | O | \Psi_v \rangle}{\langle \Psi_v | \Psi_v \rangle} \\ &= \frac{\langle \Phi_v | \{1 + S_v^\dagger\} \overline{O} \{1 + S_v\} | \Phi_v \rangle}{\{1 + S_v^\dagger\} \overline{N}_0 \{1 + S_v\}} \\ &= \frac{\langle \Phi_v | \{1 + S_{1v}^\dagger + S_{2v}^\dagger\} \overline{O} \{1 + S_{1v} + S_{2v}\} | \Phi_v \rangle}{\{1 + S_{1v}^\dagger + S_{2v}^\dagger\} \overline{N}_0 \{1 + S_{1v} + S_{2v}\}} \quad (2.17) \end{aligned}$$

where O is any of the operator, $\overline{O} = (e^{T^\dagger} O e^T)$ and $\overline{N}_0 = e^{T^\dagger} e^T$. Generally, both \overline{O} and \overline{N}_0 in the RCC approach are non-terminative series. However, we use a special trick to obtain their almost all the leading order contributions using the Wick's generalized theorem [34]. In this procedure, we evaluate first effective one-body, two body terms etc. step by step and at the end sandwich them between the S_v and its conjugate operators. This procedure has already been demonstrated in our earlier works [15, 23, 35, 36]. We also explicitly present contributions from the normalization factors evaluating them in the following way

$$Norm = \langle \Psi_v | O | \Psi_v \rangle \left\{ \frac{1}{1 + N_v} - 1 \right\}, \quad (2.18)$$

where $N_v = \{1 + S_{1v}^\dagger + S_{2v}^\dagger\} \overline{N}_0 \{1 + S_{1v} + S_{2v}\}$.

III. RESULTS AND DISCUSSIONS

Earlier, we have studied behavior of the electron correlation effects in the magnetic dipole hyperfine structure constants in the considered system using the CCSD(T) method and GTOs for few low-lying states [35] and later only in the 3d $^2D_{5/2}$ state [15]. Due to the limitations with the available computational resources at that time, we had restricted our calculations by considering only up to f-symmetry (orbital quantum number $l = 3$) orbitals. Again, we had used basis along with g-symmetry orbitals in the latter to find out the peculiar behavior of the core-polarization effects in the $^2D_{5/2}$ states of the alkaline

TABLE I: Results of A_{hfs} , B_{hfs}/Q_{nuc} and B_{hfs} of many states in $^{43}\text{Ca}^+$.

	A_{hfs}		B_{hfs}/Q_{nuc}		B_{hfs}	
	Calc (MHz)	Expt (MHz)	Calc (MHzb $^{-1}$)	Expt (MHz)	Calc (MHz)	Expt (MHz)
4s $^2S_{1/2}$	-806.387(1.0) ^a		-797.5(2.4) ^e			
	-805.348 ^b		-805(2) ^f			
	-819 ^c		-817(15) ^g			
	-794.7 ^d					
5s $^2S_{1/2}$	-234.0(2.0) ^a					
4p $^2P_{1/2}$	-145.422(340) ^a		-158.0(3.3) ^e			
	-143.068 ^b		-145.5(1.0) ^f			
	-148 ^c		-142(8) ^h			
	-144.8 ^d		145.4(0.1) ⁱ			
5p $^2P_{1/2}$	-49.651(521) ^a					
4p $^2P_{3/2}$	-30.370(415) ^a		-29.7(1.6) ^e		151.246(752) ^a	
	-30.498 ^b		-31.9(2) ^f		151.798 ^b	
	-30.9 ^c		-31.0(2) ⁱ		155 ^c	
	-29.3 ^d					
5p $^2P_{3/2}$	-10.335(112) ^a				50.904(571) ^a	
3d $^2D_{3/2}$	-47.282(289) ^a		-48.3(1.6) ^h		67.280(688) ^a	
	-47.824 ^b		-47.3(2) ⁱ		68.067 ^b	
	-52 ^c				68 ^c	
	-49.4 ^d					
	-47.27 ^j				72.06 ^j	
4d $^2D_{3/2}$	-9.474(042) ^a				17.442(134) ^a	
3d $^2D_{5/2}$	-3.622(327) ^a		-3.8(6) ⁱ		95.472(1.276) ^a	-3.9(6.0) ⁱ
	-3.552 ^b		-3.8931(2) ^k		100.208 ^b	-4.241(4) ^k
	-5.2 ^c				97 ^c	
	-4.2 ^d					
	-4.84 ^j				102.45 ^j	
4d $^2D_{4/2}$	-2.971(035) ^a				24.769(213) ^a	

^aThis work; ^b[38]; ^c[39]; ^d[40]; ^e[41]; ^f[30]; ^g[42]; ^h[43]; ⁱ[44]; ^j[22] and ^k[31].

earth-metal ions, however detail investigations in the accuracy of the wave functions for other low-lying states were not carried out in that work. In the present work, we use larger basis functions up to g-symmetry that produces the other properties [37] including electron affinity energies of many low-lying states matching with the experimental results.

In Table I, we present our A_{hfs} and B_{hfs}/Q_{nuc} (or B_{hfs}) results of many states along with the available theoretical values and experimental measurements. Estimated errors in our calculations are given inside the parenthesis. Considered sources of these errors are ba-

TABLE II: Breit contributions (Δ_{Br}) to the A_{hfs} and B_{hfs}/Q_{nuc} in MHz and MHzb^{-1} , respectively.

State	Δ_{Br}	
	A_{hfs}	B_{hfs}/Q_{nuc}
4s $^2S_{1/2}$	-0.697	
5s $^2S_{1/2}$	-0.214	
4p $^2P_{1/2}$	-0.115	
5p $^2P_{1/2}$	-0.063	
4p $^2P_{3/2}$	0.048	-0.242
5p $^2P_{3/2}$	0.014	-0.054
3d $^2D_{3/2}$	-0.102	0.150
4d $^2D_{3/2}$	0.135	-0.231
3d $^2D_{5/2}$	-0.102	0.385
4d $^2D_{5/2}$	-0.035	-0.298

sically two folds: (a) numerical calculations with limitations over finite size basis functions within g-symmetry and (b) approximations at the level of excitations in the RCC approach. In the first case, we have tested our DF results for a set of basis functions to achieve consistent results and possible discrepancies in these results are assumed as one of the sources of errors. Second, we approximate our level of excitations at the singles and doubles as Ca^+ is assumed as not too heavy system. However, equations to determine these amplitudes, in principle, should couple with the higher excitations for accurate calculations. Although our leading order triple excitations take care of most of these contributions, we estimate the contributions from the higher excitations by studying differences of results between the CCSD and CCSD(T) methods and evaluating lower order diagrams that may arise through the neglected triple excitations in the RCC approach. This procedure may not be sufficient enough, however it explains their importance qualitatively. We have scaled these contributions to account as the upper values of the second source of errors.

It is obvious that our A_{hfs} results match quite well within the uncertainties of available experimental values giving an indication that our calculated wave functions are accurate enough in the nuclear region. There are also experimental results available for B_{hfs} in many cases, but none of them are accurate enough except the recent measured value in the 3d $^2D_{5/2}$ state [31]. It is obvious from Table I that there are quite well agreement between different calculations of B_{hfs}/Q_{nuc} results at least in the 4p $^2P_{3/2}$ and 3d $^2D_{3/2}$ states, but there comes large discrepancies between the results in the 3d $^2D_{5/2}$ state. Due to consistency among the theoretical calculations in the 4p $^2P_{3/2}$ and 3d $^2D_{3/2}$ states, it would indeed be appropriate to combine these results with the measured B_{hfs} values of their corresponding states to determine less accurately known Q_{nuc} in ^{43}Ca . In contrast, B_{hfs} of the 3d $^2D_{5/2}$ state is measured quite precisely and hence it is necessary to use its calculated B_{hfs}/Q_{nuc} result to combine with

its measured B_{hfs} value to determine Q_{nuc} in the considered system. Therefore, we would like to investigate possible reasons of the discrepancies among the theoretical methods which are employed in these calculations. First, we investigate the role of the Breit interaction from which we can realize the effect of higher relativistic effects in the above properties which was not considered in the previous works, then we proceed with describing differences in the inclusion of various electron correlation effects through the employed theoretical methods.

For high accuracy calculations, it may be necessary to find out contributions from higher order relativistic corrections than the Coulomb interaction; occurs through the exchange of longitudinal photons. The next important contribution from frequency independent Breit interaction due to the transverse photon [45] can be assumed as a bench mark test to estimate how big the neglected relativistic effects would be. In Table II, we present contributions from the Breit interaction in the A_{hfs} and B_{hfs}/Q_{nuc} calculations for different states. As seen, these contributions in the considered system are not large and it is larger in the ground state than in the excited states. It seems from this study that higher order relativistic corrections like bound state QED effects are not important for high precision calculations in the present system and the results mostly depend on the electron correlation effects.

We now discuss the differences between various works that account correlation effects at various level of orders. As mentioned earlier, our previous and present works are carried out with all order RCC method, but the main differences in the results are due to inclusion of orbitals from g-symmetry and Breit interaction in this work. Both Yu et al. [38] and Martensson et al. [39] have carried out their calculations using semi-empirical feature many-body methods. They contain all order core-polarization effects, however other correlation effects like Bruckner pair correlation effects [34] are taken up to certain orders. In the work of Yu et al., they have restricted orbitals in the evaluation of the hyperfine structure constants for individual state by selecting maximum contributing angular momentum configurations. However, contributions from all these orbitals are intrinsically accounted through the coupled equations in the RCC method. In Tables III and IV, we present contributions from individual RCC terms to our A_{hfs} and B_{hfs}/Q_{nuc} results, respectively. As seen our DF results match well with the Martensson et al., but there are differences between all order core-polarization contributions between their work and ours. Our all order core-polarization effects are associated with the S_{2v} RCC operator [35, 36]. The reason of discrepancies could be due to the fact that all correlation effects are coupled in the RCC method in contrast to the above semi-empirical features. There is also one non-relativistic theory with relativistic corrections under random phase approximation (RPA) approach has been employed [40] for calculating these hyperfine structure constants. Recently, another calculation has been carried out using

TABLE III: RCC contributions to the A_{hfs} calculations.

RCC terms	$4s\ ^2S_{1/2}$	$5s\ ^2S_{1/2}$	$4p\ ^2P_{1/2}$	$5p\ ^2P_{1/2}$	$4p\ ^2P_{3/2}$	$5p\ ^2P_{3/2}$	$3d\ ^2D_{3/2}$	$4d\ ^2D_{3/2}$	$3d\ ^2D_{5/2}$	$4d\ ^2D_{5/2}$
O (DF)	-587.902	-181.120	-101.559	-36.396	-19.669	-7.056	-33.409	-8.104	-14.235	-3.455
$O - \overline{O}$	-1.626	0.111	1.076	0.370	0.215	0.080	-0.604	-0.079	-0.283	-0.041
$\overline{O}S_{1v} + cc$	-103.321	-21.064	-21.032	-5.887	-4.089	-1.159	-8.373	-0.244	-3.554	-0.100
$\overline{O}S_{2v} + cc$	-102.224	-28.843	-19.997	-6.345	-5.386	-1.812	-3.120	-0.926	15.803	1.138
$S_{1v}^\dagger \overline{O}S_{1v}$	-4.527	-0.613	-1.113	-0.245	-0.217	-0.049	-0.571	-0.031	-0.241	-0.013
$S_{1v}^\dagger \overline{O}S_{2v} + cc$	-7.338	-0.873	-1.689	-0.313	-0.374	-0.048	-0.260	0.115	0.932	-0.112
$S_{2v}^\dagger \overline{O}S_{2v} + cc$	-9.615	-3.117	-1.108	-0.355	-0.837	-0.348	-2.017	-0.384	-2.125	-0.443
$Norm$	8.466	1.519	1.107	0.273	0.232	0.057	1.072	0.179	0.081	0.055

TABLE IV: RCC contributions to the B_{hfs}/Q_{nuc} calculations.

RCC terms	$4p\ ^2P_{3/2}$	$5p\ ^2P_{3/2}$	$3d\ ^2D_{3/2}$	$4d\ ^2D_{3/2}$	$3d\ ^2D_{5/2}$	$4d\ ^2D_{5/2}$
O (DF)	96.976	34.789	55.354	13.354	78.466	18.939
$O - \overline{O}$	-0.869	-0.307	3.208	0.493	4.456	0.680
$\overline{O}S_{1v} + cc$	20.220	5.736	15.275	0.306	21.509	0.451
$\overline{O}S_{2v} + cc$	32.885	10.217	-5.066	2.836	-6.843	4.067
$S_{1v}^\dagger \overline{O}S_{1v}$	1.076	0.243	1.155	0.060	1.619	0.084
$S_{1v}^\dagger \overline{O}S_{2v} + cc$	1.770	0.286	-1.586	0.456	-2.225	0.632
$S_{2v}^\dagger \overline{O}S_{2v} + cc$	0.341	0.220	0.621	0.308	0.844	0.432
$Norm$	-1.153	-0.280	-1.681	-0.371	-2.354	-0.516

TABLE V: Comparison of Q_{nuc} values (in b) from various works.

Q_{nuc}	Reference
-0.0444(6)	This work
-0.040(8)	[10]
-0.0408(8)	[26]
-0.043(9)	[30]
-0.065(20)	[28]
-0.049(5)	[29, 47]
-0.044	[38]
-0.062(12)	[48]

TABLE VI: Calculations of B_{hfs} (in MHz) using new Q_{nuc} value and our B_{hfs}/Q_{nuc} results reported in Table I.

State	B_{hfs}
$4p\ ^2P_{3/2}$	-6.715(125)
$5p\ ^2P_{3/2}$	-2.260(56)
$3d\ ^2D_{3/2}$	-2.987(71)
$4d\ ^2D_{3/2}$	-0.774(16)
$3d\ ^2D_{5/2}$	-4.239(115)
$4d\ ^2D_{5/2}$	-1.100(24)

multi-configurational Dirac-Fock (MCDF) method [22]. In contrast to our RCC approach, these methods account less correlation effects at the same level of excitations.

As seen in Tables III and IV, the trend of correlation effects in A_{hfs} calculations in the first five low-lying states are same as discussed in our previous works [15, 35] except the differences in the magnitudes are due to the new basis functions. The amount of correlation effects in the higher excited states are comparatively smaller. Likewise in A_{hfs} , both the pair correlation and core-polarization effects which arise through S_{1v} and S_{2v} RCC operators [15, 35], respectively, play major roles in obtaining the final results of B_{hfs}/Q_{nuc} . The differences between our B_{hfs}/Q_{nuc} result of the $3d\ ^2D_{5/2}$ state with others is due to the accurate treatment of these correlation ef-

fects in the present work. Combining our B_{hfs}/Q_{nuc} result with the measured B_{hfs} value of this state [31], we get $Q_{nuc} = -0.0444(6)b$. Following the same procedure when we combine B_{hfs}/Q_{nuc} results of the $4p\ ^2P_{3/2}$ and $3d\ ^2D_{3/2}$ states with their corresponding experimental B_{hfs} results, it gives less accurate values as $Q_{nuc} = -0.044(10)b$ and $Q_{nuc} = -0.059(29)b$, respectively. The associated larger errors are mainly due to larger uncertainties in the experimental results. We compare the above accurately estimated Q_{nuc} value with the previously reported results in Table V. Our result is around 10% improvement over the considered standard value $-0.044(5)b$ [46] in this system. Recently Yu et al. [38] had evaluated this value as $-0.044b$, which is compatible with our result, by combining their B_{hfs}/Q_{nuc} result of the $4p\ ^2P_{3/2}$ state with its experimental B_{hfs} value which has around 20% uncertainty. Sundholm and

TABLE VII: Hyperfine interaction energies (W_F) for different $|F; I, J\rangle$ states in $^{43}\text{Ca}^+$ in MHz.

$F \backslash JM_J\rangle$	4s $^2S_{1/2}$	5s $^2S_{1/2}$	4p $^2P_{1/2}$	5p $^2P_{1/2}$	4p $^2P_{3/2}$	5p $^2P_{3/2}$	3d $^2P_{3/2}$	4d $^2P_{3/2}$	3d $^2P_{5/2}$	4d $^2D_{5/2}$
1									38.477	32.834
2					201.400	68.551	317.553	63.535	32.444	27.207
3	1814.371	526.500	327.201	111.715	115.087	39.160	177.841	35.666	22.940	18.647
4	-1411.177	-409.500	-254.489	-86.889	-4.475	-1.534	-10.434	-2.009	9.421	7.015
5					-161.121	-54.824	-248.977	-49.932	-8.840	-7.880
6									-32.752	-26.271

Olsen [26] had combined precisely measured B_{hfs} of the 3d 4s 1D_2 state of ^{43}Ca with their calculated electric field gradient result to obtain $Q_{nuc} = -0.0408(8)b$ in the same atom. In this work, they had employed the MCDF method on the restricted active space to calculate electric field gradient. We have already discussed the difference between the RCC and MCDF methods earlier in this section. There are also other works [10, 28, 29, 30, 47, 48] finding Q_{nuc} in ^{43}Ca , but all of them have used either large uncertainty experimental results or more approximated theoretical methods like second order many-body perturbation theory, results correcting for Sternheimer effects using the anti-shielding factor in the Hartree-Fock calculations etc. that cope with lesser electron correlation effects than our RCC method.

Using our new Q_{nuc} value, we determine B_{hfs} from our B_{hfs}/Q_{nuc} results presented in Table I and have given them in Table VI. The new B_{hfs} results are well within the error bars of experimental values with less uncertainties. Again, we evaluate energies of different hyperfine states using the formula given by Eq. (2.2) corresponding to each fine structure level. In Table VII, we have reported these results which can be verified by analyzing isotope shift measurements in the future experiments in the assumed system.

IV. CONCLUSION

We have employed the relativistic coupled-cluster method in the Coulomb and Breit interaction approximation to calculate the atomic wave functions in $^{43}\text{Ca}^+$. Using these wave functions, we were able to determine A_{hfs} and B_{hfs}/Q_{nuc} results accurately. By combining our B_{hfs}/Q_{nuc} result of the 3d $^2D_{5/2}$ state with its corresponding precisely measured B_{hfs} value, we determine Q_{nuc} of ^{43}Ca as $-0.0444(6)b$ which is 10% improvement over the considered standard value. In this work, we have also given contributions separately from the Breit interaction and hyperfine interaction energies for a number of states. Our new Q_{nuc} value and reported hyperfine interaction energies may serve the researcher of both atomic and molecular physics.

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